Agilent 7890 GC and 7000B GC/MS/MS Presentation for CA Dept of Toxic Substances Control Environmental Chemistry Laboratory
Jan 26, 2011

Agilent Technologies
Tim Borrego
Account Manager
Santa Clara, CA

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Agenda

- Why MS/MS?

- Hardware Features of 7000B MS/MS

- Hardware Features of 7890 GC that help mass spec

- Software

- Applications

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Why MS/MS?
Greater Selectivity Than SIM

EI-SIM
Selectivity proportional to spectral resolution
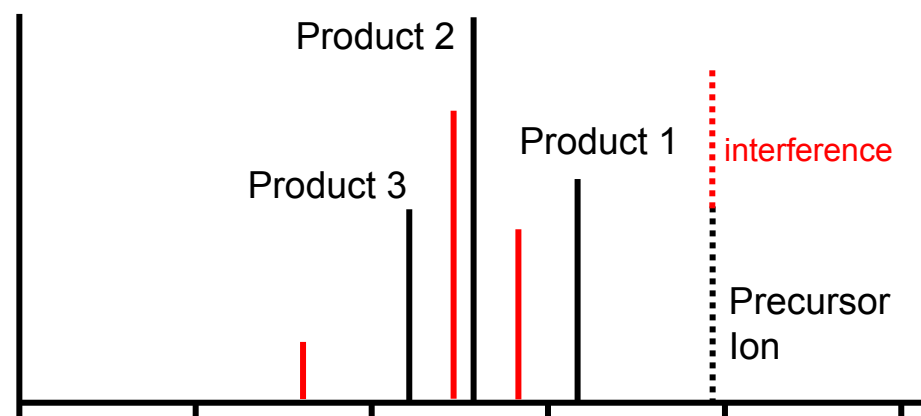
No selectivity against ions with same m/z

unit mass resolution

interference

analyte

EI-MS/MS
Precursor selectivity same as SIM
High probability that at least one product ion will be a unique dissociation product of the precursor BUT not the interference
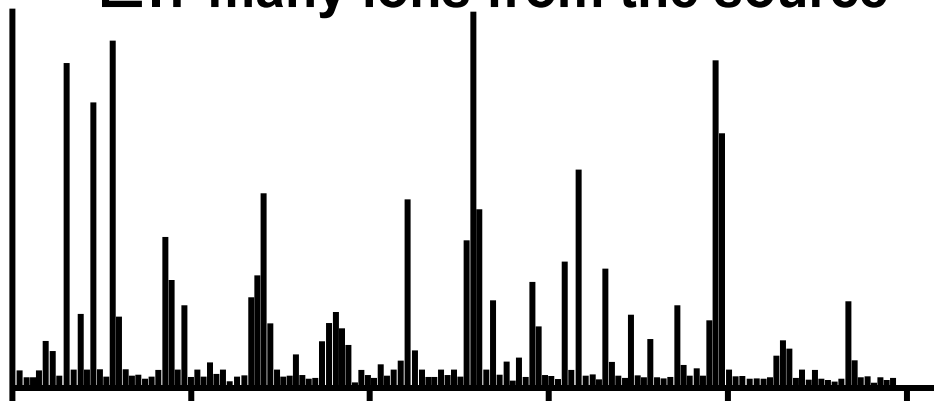
Product 2

Product 1

Product 3

interference

Precursor Ion

The precursor ion should ***NOT*** be used for ion ratios or quantitation since the interferences will be the same as the SIM ion
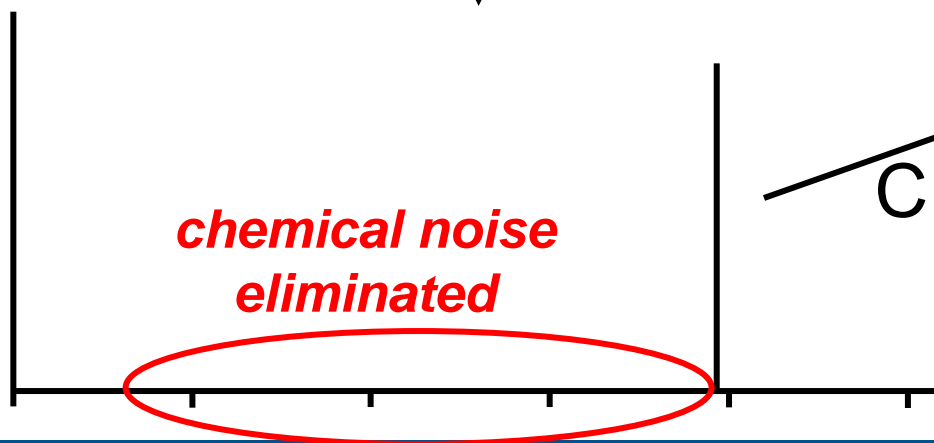
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Why MS/MS?
Lower detection limits by reducing noise
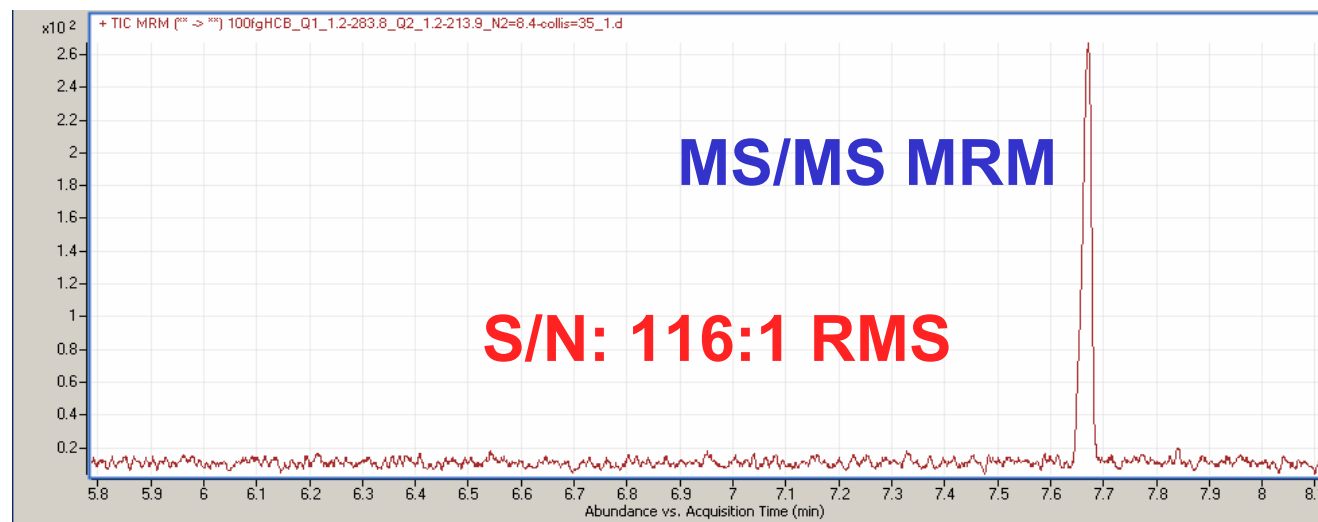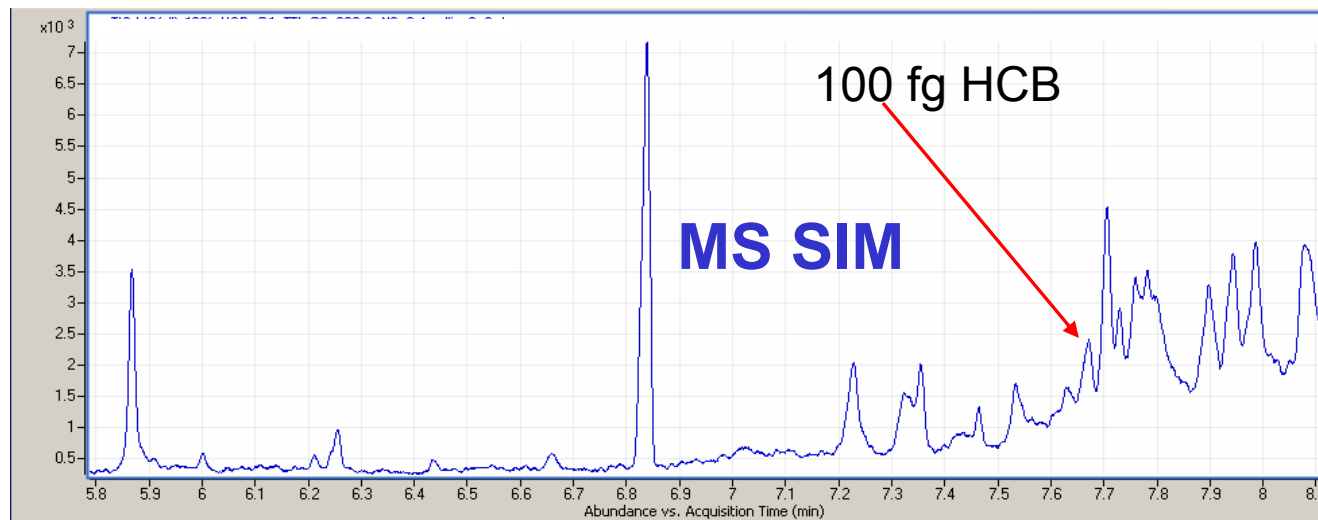
EI: **many ions from the source**

Product ion signal often decreases, but the percentage decrease in noise is much larger for real samples; S/N and detection limits improve

Q1 SIM **isolate precursor before CID**

CID + Q2 SIM

chemical noise eliminated

Product 2

Product 3

Product 1

Product ion measured against zero chemical noise

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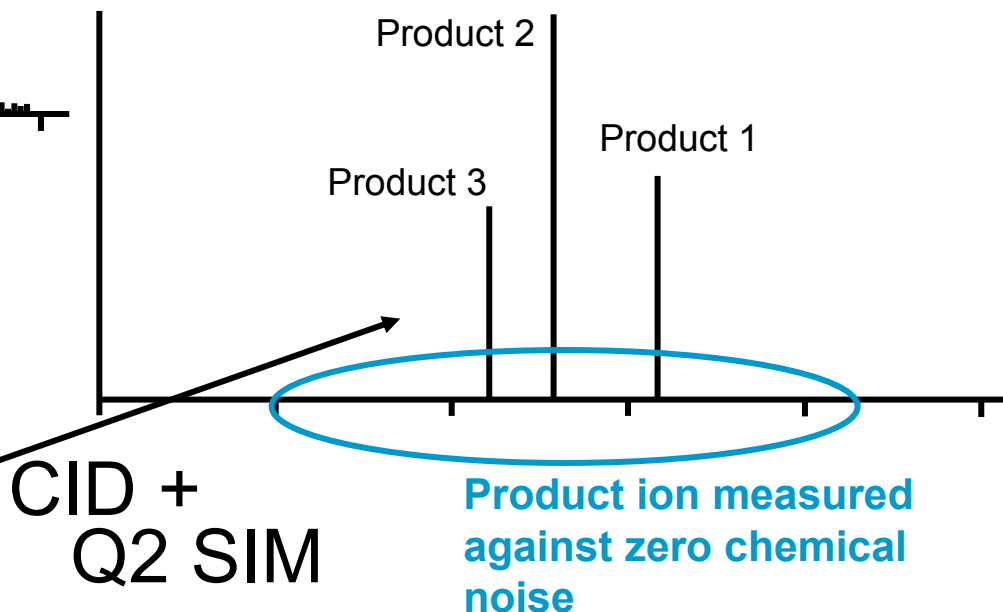
Why GC/MS/MS?
A Picture Is Worth a Thousand Words

GC/MS Single Quad SIM

100 fg HCB

MS SIM

GC/MS/MS MRM

EI 100fg HCB in "DIRTY" Matrix

MS/MS MRM

S/N: 116:1 RMS

A chromatographer's dream: single peak on flat baseline

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Technology

Agilent took the best technologies from their industry leading 5975 GC/MSD:

- – Heated monolithic gold plated quartz quadrupole
- – Proven reliable high performance source design
- – AUTOTUNE

and the 6400 Series LC/MS/MS:

- – Linear acceleration enhanced Collision Cell
- – Wide Mass-Bandwidth MS/MS ion optics
- – Mass Hunter software

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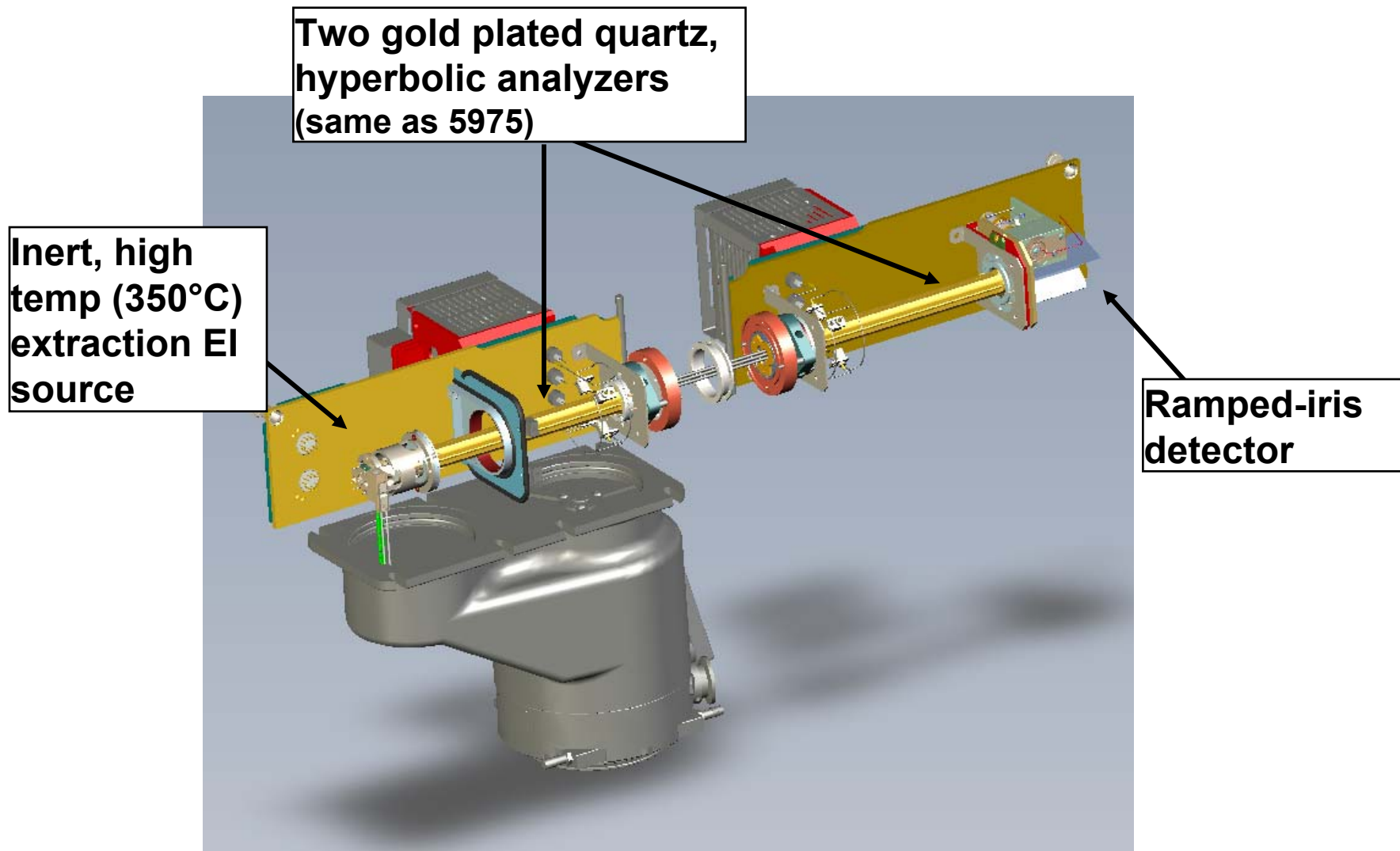
Why Heated Quartz "Gold" Quads?

Unlike LC/MS, many high boiling neutral molecules enter the source and manifold of a GC/MS or GC/MS/MS

- Higher temperature reduces potential for contamination
  - 200C max
  - Virtually eliminates the need to clean quads
- Low coefficient for thermal expansion for quartz
  - Stable structure during maintenance cycles (hot-cool-hot) for source or detector

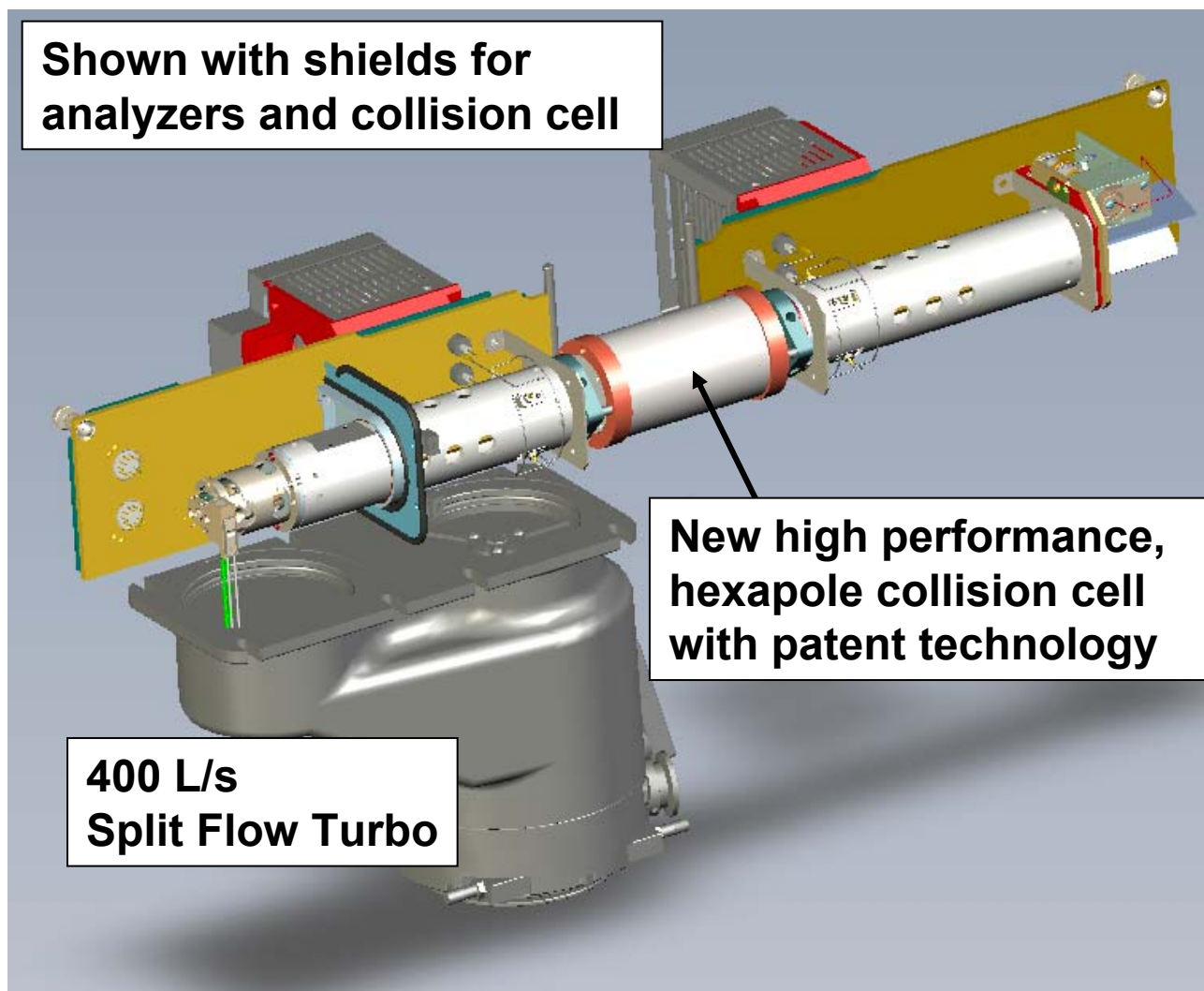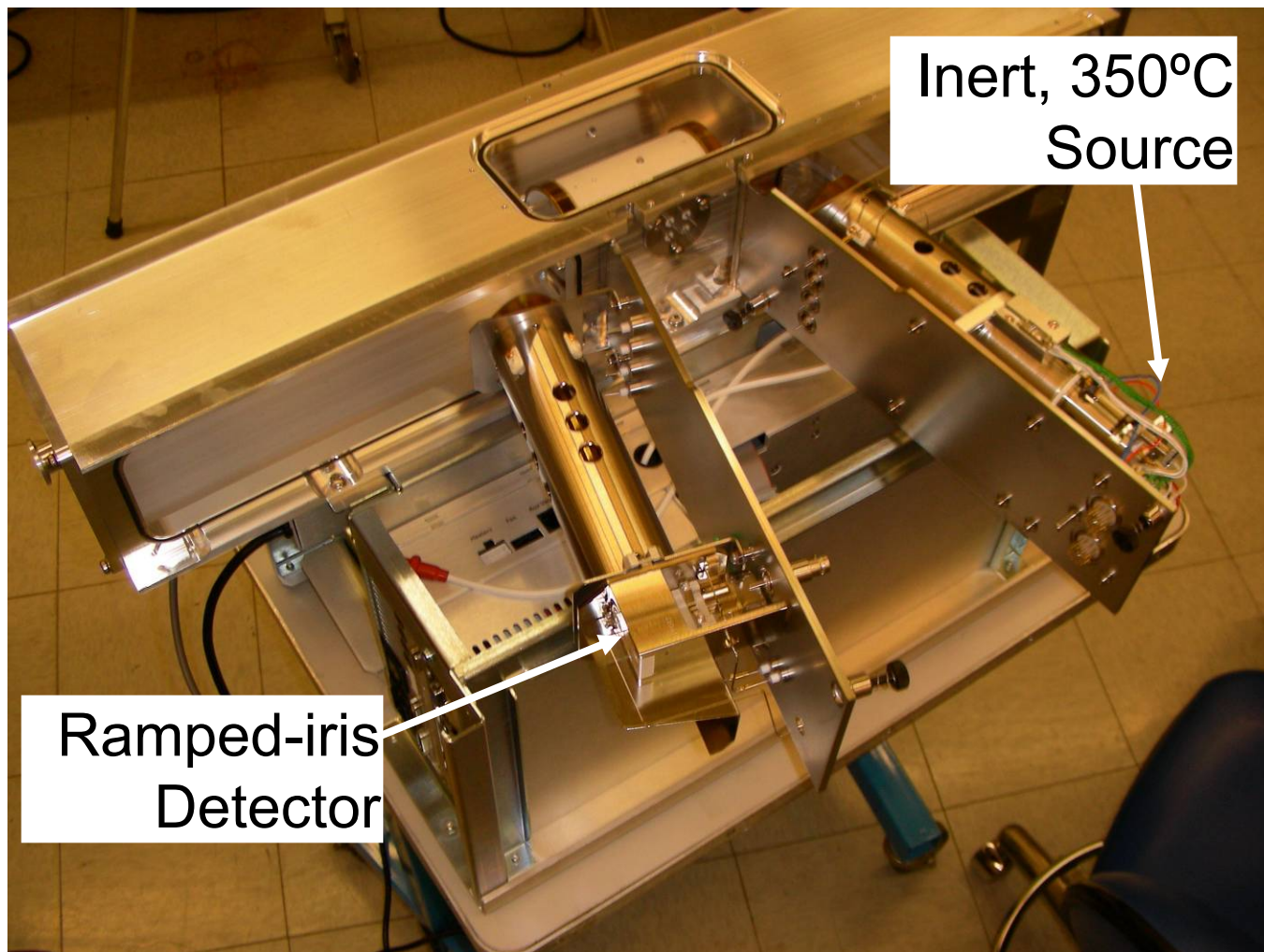More stable tunes and methods over a longer period of time in real world sample environments

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GC/MS/MS Analyzer

Two gold plated quartz, hyperbolic analyzers (same as 5975)

Inert, high temp (350°C) extraction EI source

Ramped-iris detector

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GC/MS/MS Analyzer

Shown with shields for analyzers and collision cell

New high performance, hexapole collision cell with patent technology

400 L/s Split Flow Turbo

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Analyzer Doors Open

Inert, 350ºC Source

Ramped-iris Detector

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Proven Inert Source Performance

Stay-Clean design extends maintenance intervals with dirty samples

Can be heated to 350°C

Has both repeller and extraction technologies to increase ion flux into the mass analyzer

Source tune parameters in the Autotune file

Dual filament design reduces maintenance intervals

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High Performance Collision Cell Design

Linear acceleration design is optimized for high speed performance without ion ghosting or cross-talk

MRM speed to 500 MRMs/sec allows determination of more compounds per ion group

High sensitivity with wide mass bandwidth eliminates the need to "tune on your compound" for optimum sensitivity

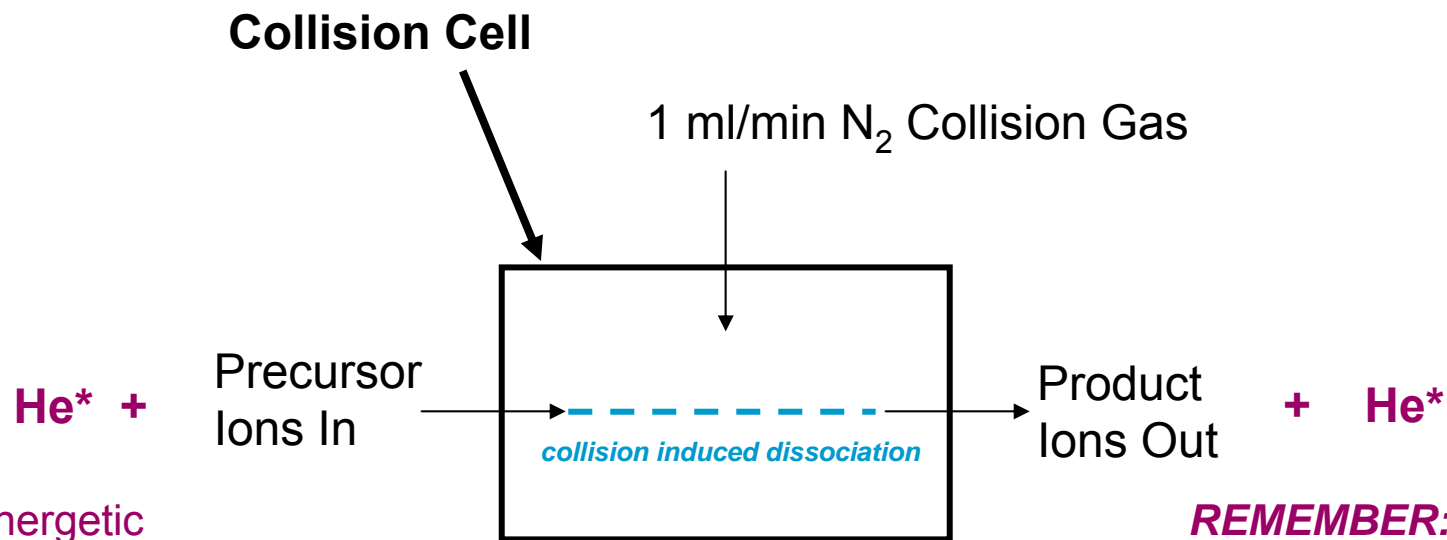**"Helium Quenching"** neutral noise reduction increases S/N

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Collision Cell Details

(Cell housing and 2 rods removed for clarity)

Quadrupole
post-filter

Support
cradle

Quadrupole
pre-filter

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Technical Advantage: Collision Cell

Collision Cell

1 ml/min N$_2$ Collision Gas

He* +   Precursor Ions In   →   *collision induced dissociation*   →   Product Ions Out   **+   He***
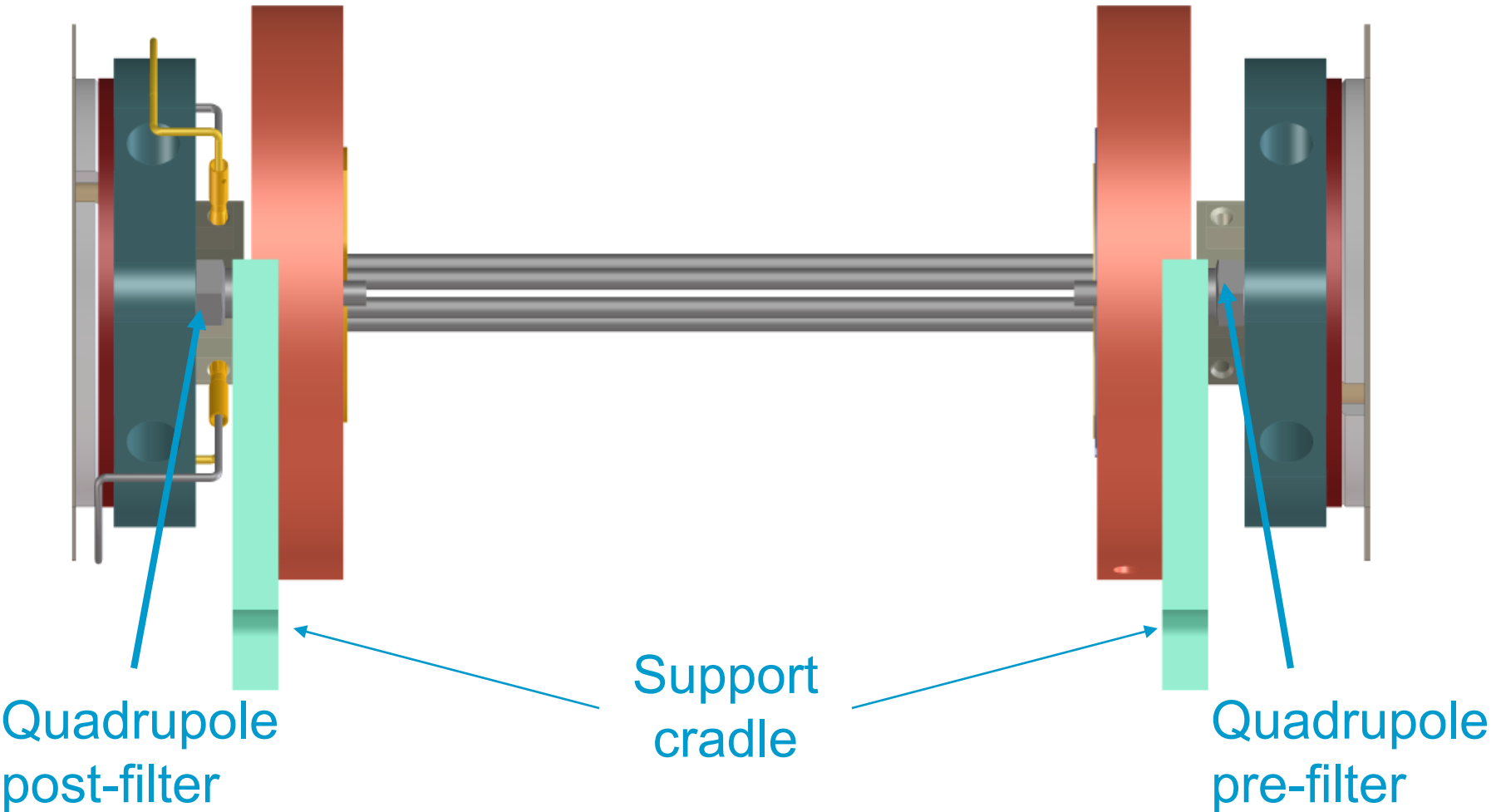
Highly energetic helium metastables are produced in an EI source and can pass through the electrical fields unaffected – producing "neutral noise" at the HED-EM.

REMEMBER:
In GC/MS, Chemical Noise is much higher than Neutral Noise.
In GC/MS/MS with the elimination of Chemical Noise, Neutral Noise is a critical source of noise.

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Technical Advantage: Collision Cell Quench Gas

Collision Cell

1 ml/min N_2 Collision Gas

He* +

Precursor Ions In

collision induced dissociation

Product Ions Out

Helium metastable neutral noise eliminated.

He Buffer Gas

He* + He $\longrightarrow$ 2 He + heat

He* + N_2 $\longrightarrow$ $N_2^{+\cdot}$ + He + e⁻

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Effect of "Helium Quench"

S/N 341:1 Helium Quench Gas OFF

S/N 1294:1 Helium Quench Gas ON
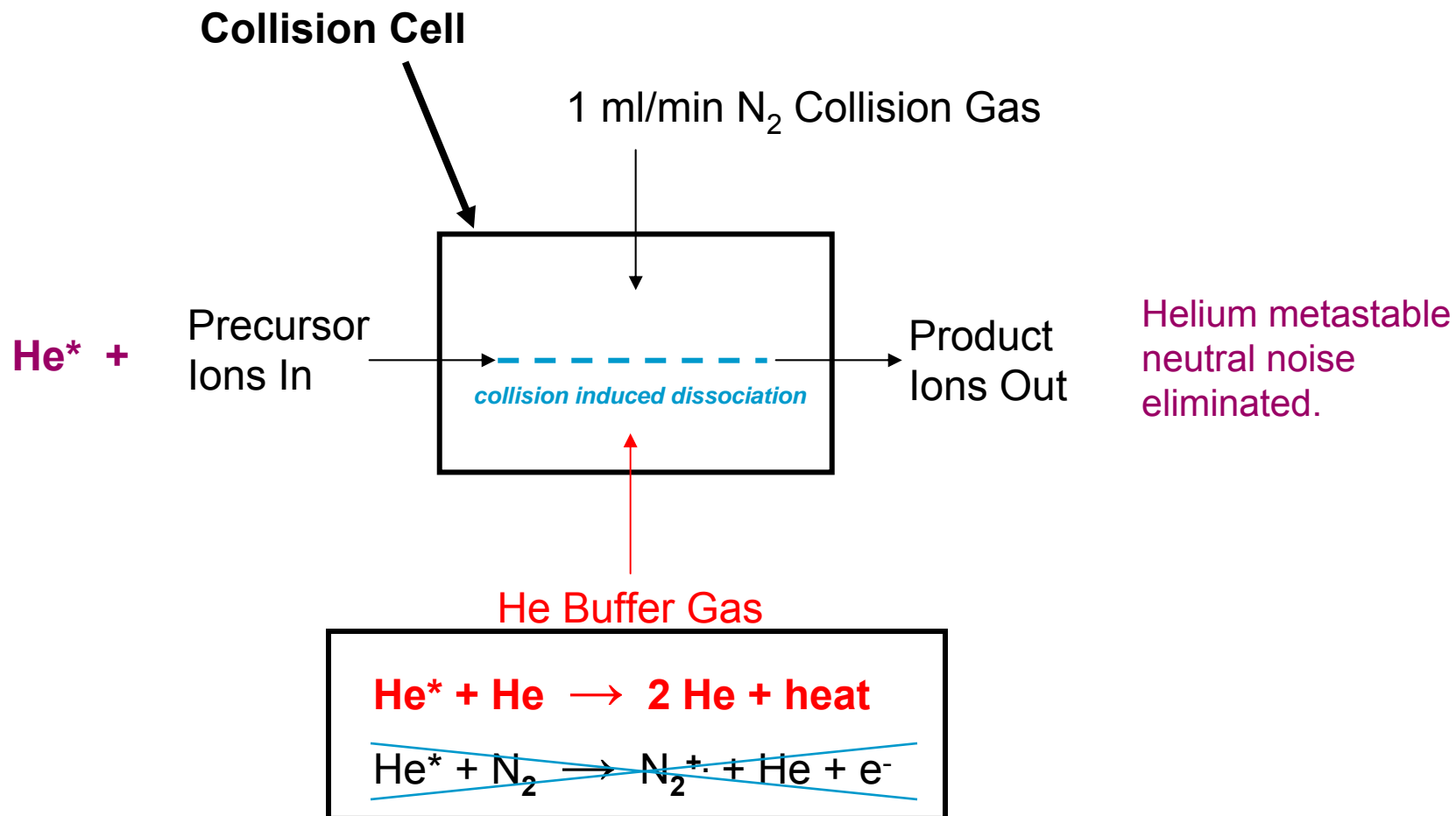
tested with hexachlorobenzene

Noise Comparison

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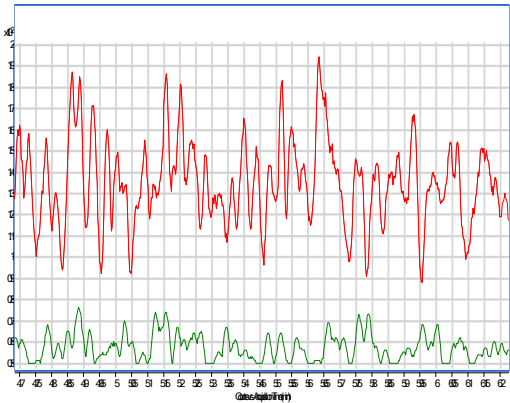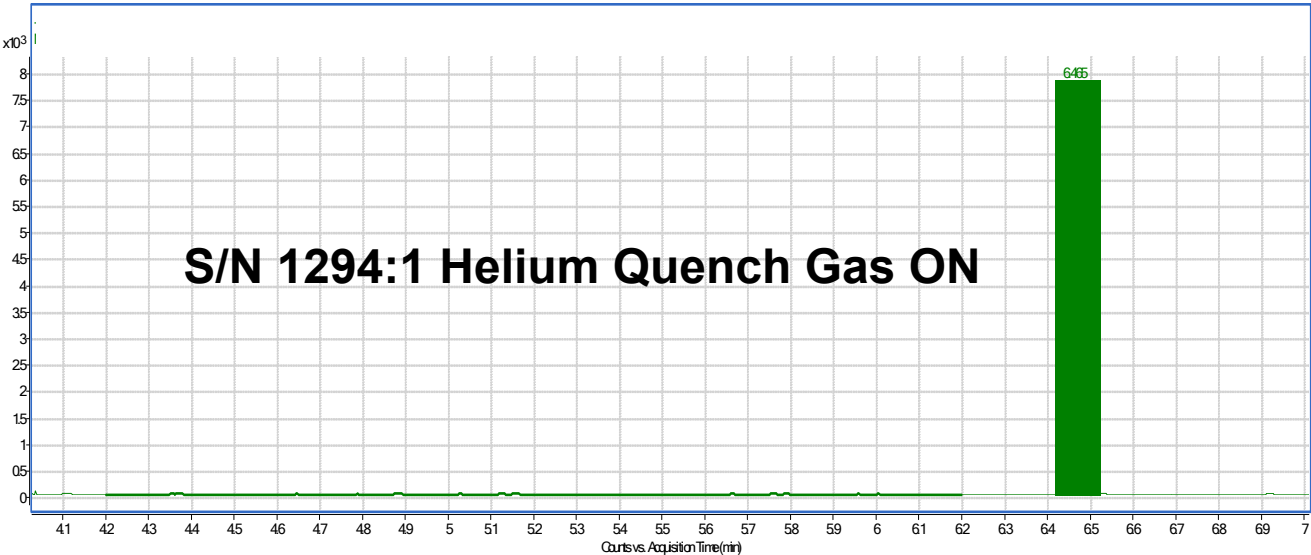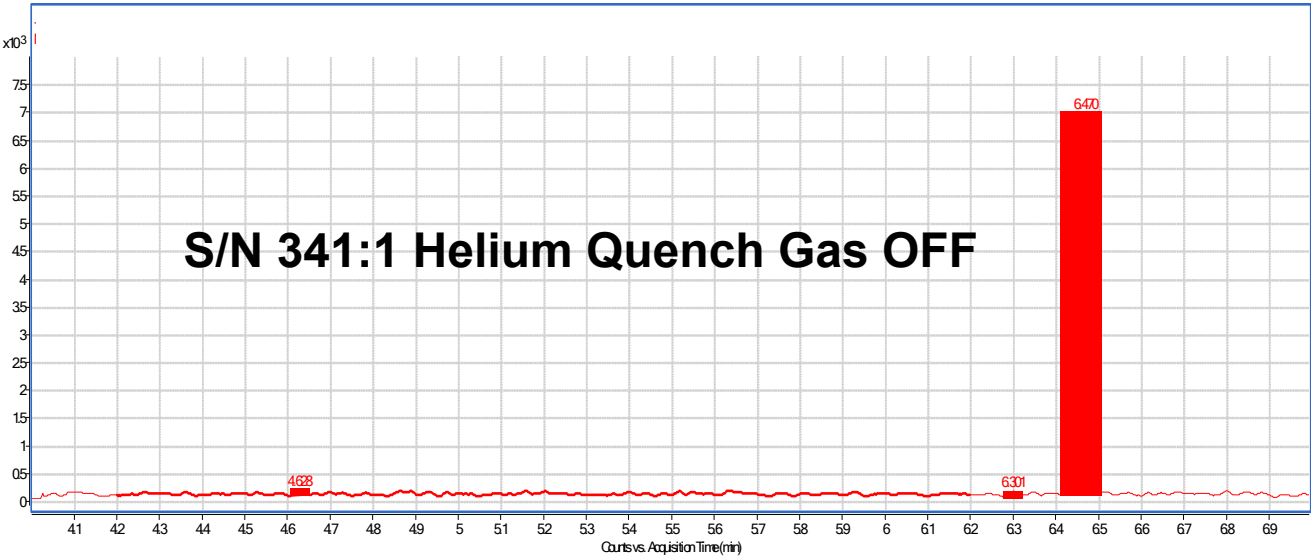
High Performance Ramped-Iris Detector

Ultra low neutrals noise

Long life and high linearity

"Gain Normalization" corrects tune file for detector aging to allow repeatable long term method sensitivity

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Ramped-Iris Detector

Offset Z

shield for secondary particles

steering rod

hyperbolic quartz transmission quadrupole analyzer

high energy dynode

ion beam

triple channel electron multiplier

Y

X

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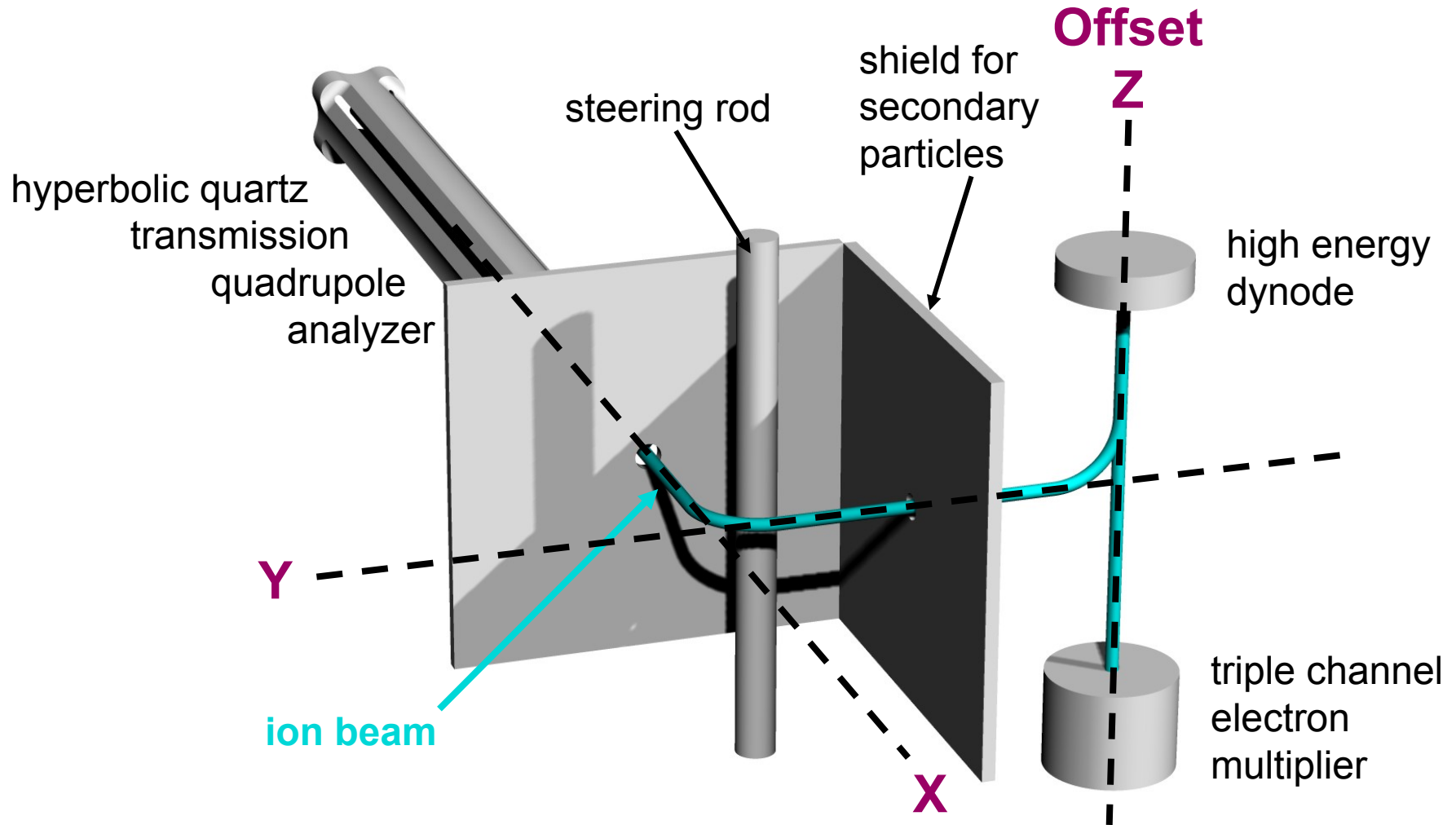
Agilent 7000B GC/MS/MS

Outstanding sensitivity 100fg of OFN on column at 500:1 S/N RMS in MS/MS mode using AUTOTUNE parameters verified at customer installation.

1050 amu Mass Range

500 MRM/sec Speed

Reliable heated monolithic gold plated hyperbolic quadrupoles

Differentially pumped vacuum system

Helium quenching collision cell technology

Agilent 7890 GC with Capillary Flow technology.

MassHunter Software

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7000B EI MRM Specifications

EI MRM Spec:

- S/N 500:1 on 100fg OFN of the 272:222 or 272:241 transition
    - Installation test: as 100fg; splitless
- 8% RSD on peak area of the 272:222 or 272:241 transition

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7000B CI Specifications

PCI MRM Spec:

- S/N 50:1 on 100fg BZP MRM of 183:105 transition

NCI SIM Spec:

- S/N 200:1 on 10fg OFN MS1 SIM of m/z 272

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Autotune

Proprietary program tunes the source, mass analyzer, and detector for (as applicable):

- Ion transmission

- Mass axis calibration

- Mass resolution

- Detector gain vs Voltage

Autotune settings are saved with the method for repeatable method performance.

Manual Tune override is available

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MassHunter MS Workstation Software

Modern software interpretation of the proven industry standard GC/MS ChemStation platform

Single software platform for all Agilent MS Systems

- LC/SQ , LC/MS/MS, LC/TOF, LC/QTOF

- GC/SQ, GC/MS/MS, GC/QTOF (future)

- ICP/MS

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New Agilent Multimode Inlet Improvements

Turn-top easy liner exchange

Standard 11mm septa

No leaks at liner

Air plus CO2, N2 cryogenic cooling
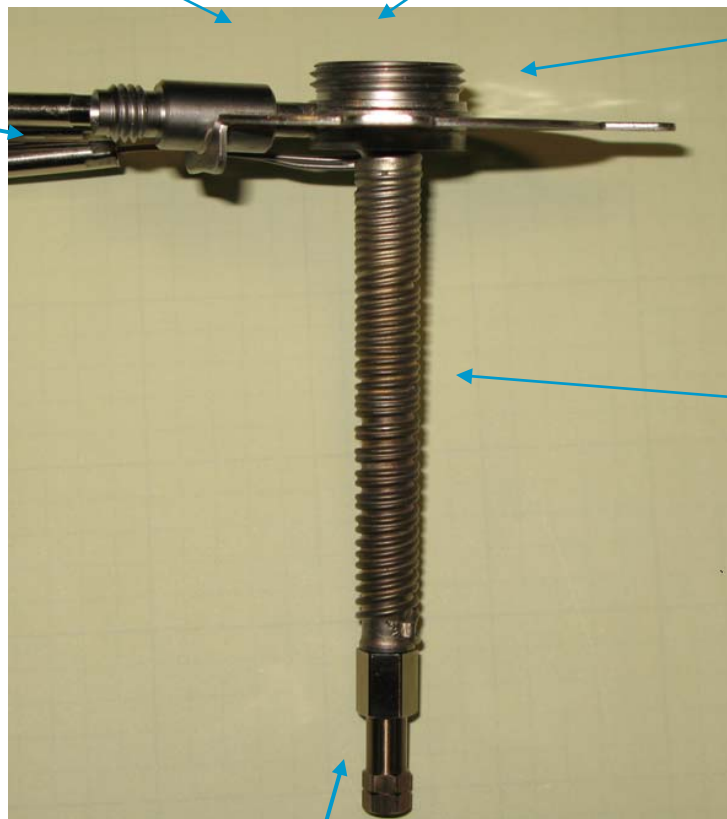
Standard liner dimensions

Standard column nut

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Agilent Multimode Inlet Features

Hardware

Temperature range of -160 to 450°C

Heating ramps as fast as 900°C/min

Septum/Liner Easily Exchangeable

Injection Modes: Hot S/SL, Cold S/SL, all in pulsed mode, solvent vent mode, residue removal mode

Support for single stroke injections from 0.1 μL to 250 μL

Software

Ten temperature ramps

Solution for solvent vent timing

Fully integrated into ChemStation, MSD ChemStation, EZChrom, MassHunter

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Large Volume (LVI) Injection of Triazine Herbicides
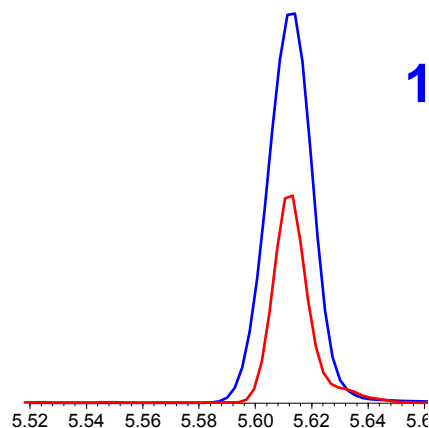
1µL Cold Splitless inj

1µL Hot Splitless inj
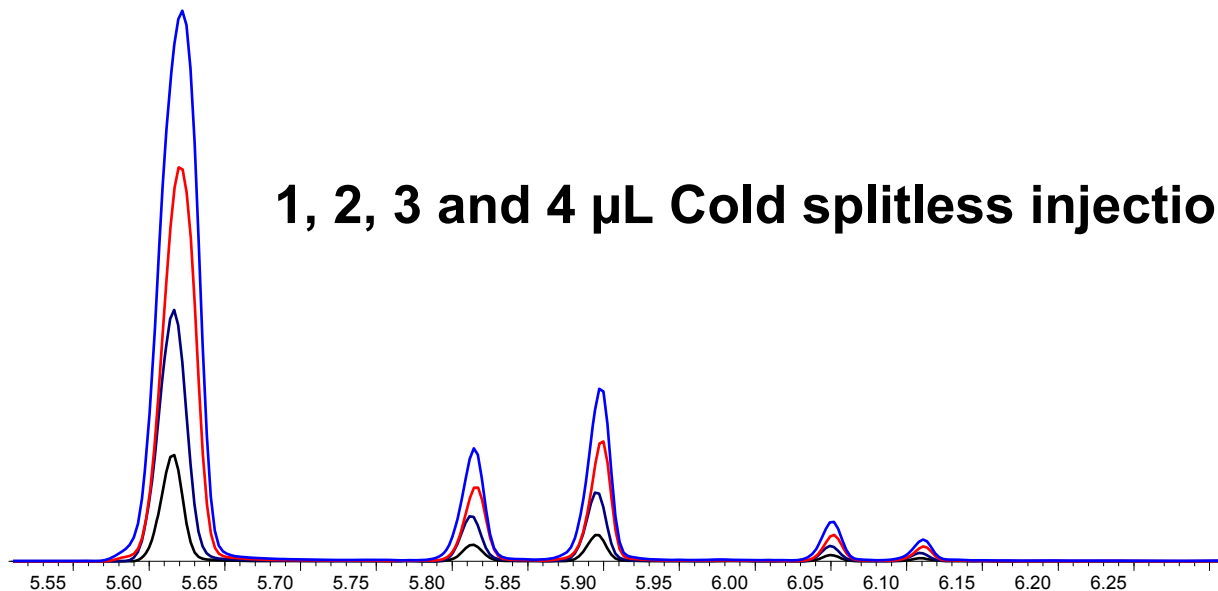
1, 2, 3 and 4 µL Cold splitless injections (ethyl acetate)

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Backflush: Many Advantages for GC/MS Analysis of Complex Samples ('Dirty Matrices')

- Provides more consistent GC retention times

- Provides better, more consistent MS spectra through a sample sequence

  – Reduces chemical noise that may increase during a sequence of samples due to small carryover of matrix from sample to sample

  – Higher quality quantitation (no increase in interfering ions during analysis sequence)

- Reduces contamination (and cleaning frequency) for the source

- Reduces analysis time (more samples per day)

- Increases lifetime of analytical column

- Multiple ways to setup the backflush using Capillary Flow Technologies

  – QuickSwap, Deans Switch, 2-Way Splitter with Makeup, 3-Way Splitter with Makeup, and Purged Ultimate Union

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Without Backflush: A Serious Problem
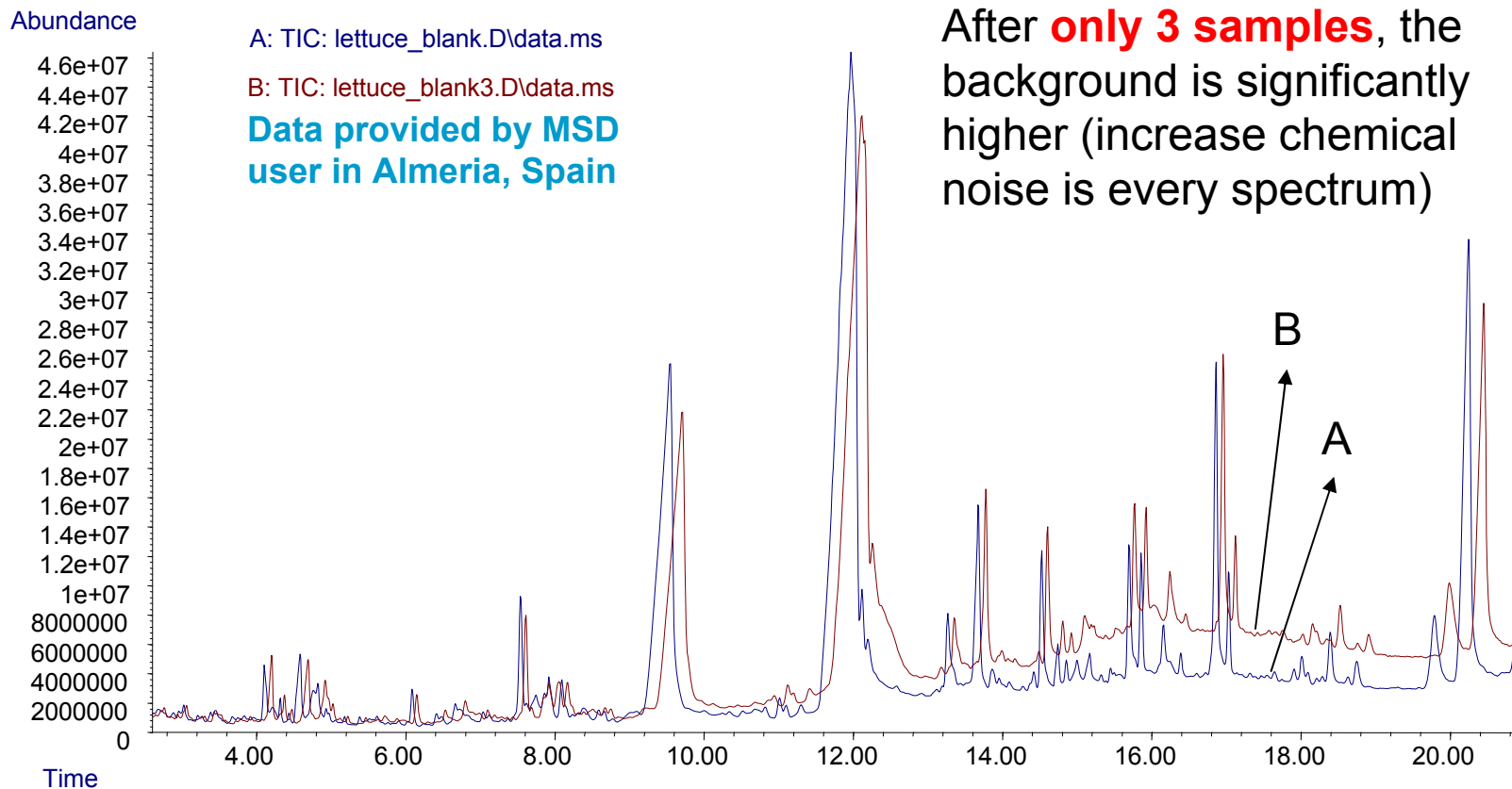
A: TIC: lettuce_blank.D\data.ms

B: TIC: lettuce_blank3.D\data.ms

Data provided by MSD user in Almeria, Spain

After **only 3 samples**, the background is significantly higher (increase chemical noise is every spectrum)

Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

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Without Backflush: Changes in Retention Time
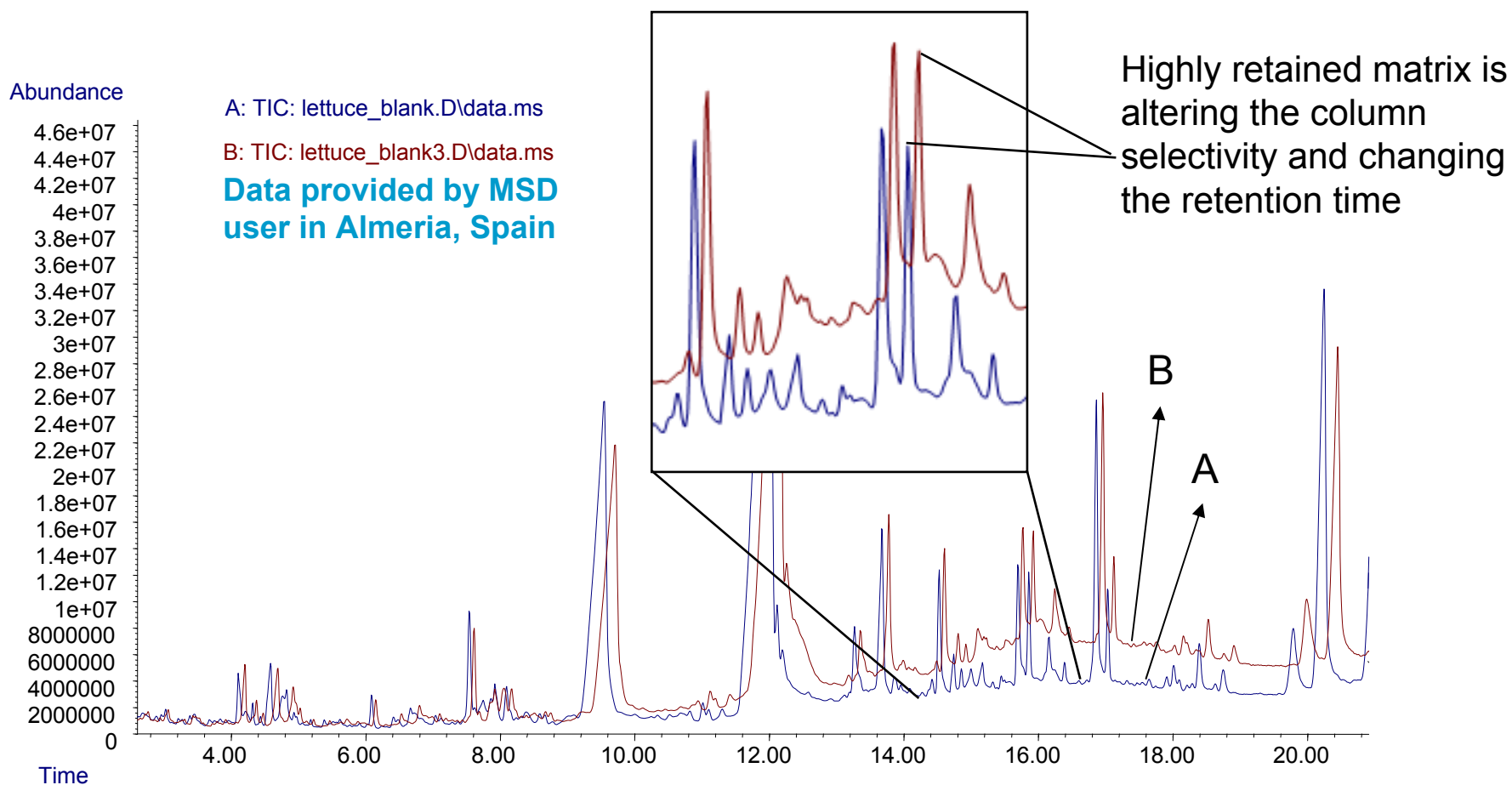
A: TIC: lettuce_blank.D\data.ms

B: TIC: lettuce_blank3.D\data.ms

Data provided by MSD user in Almeria, Spain

Highly retained matrix is altering the column selectivity and changing the retention time

Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

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Without Backflush: Increased Background
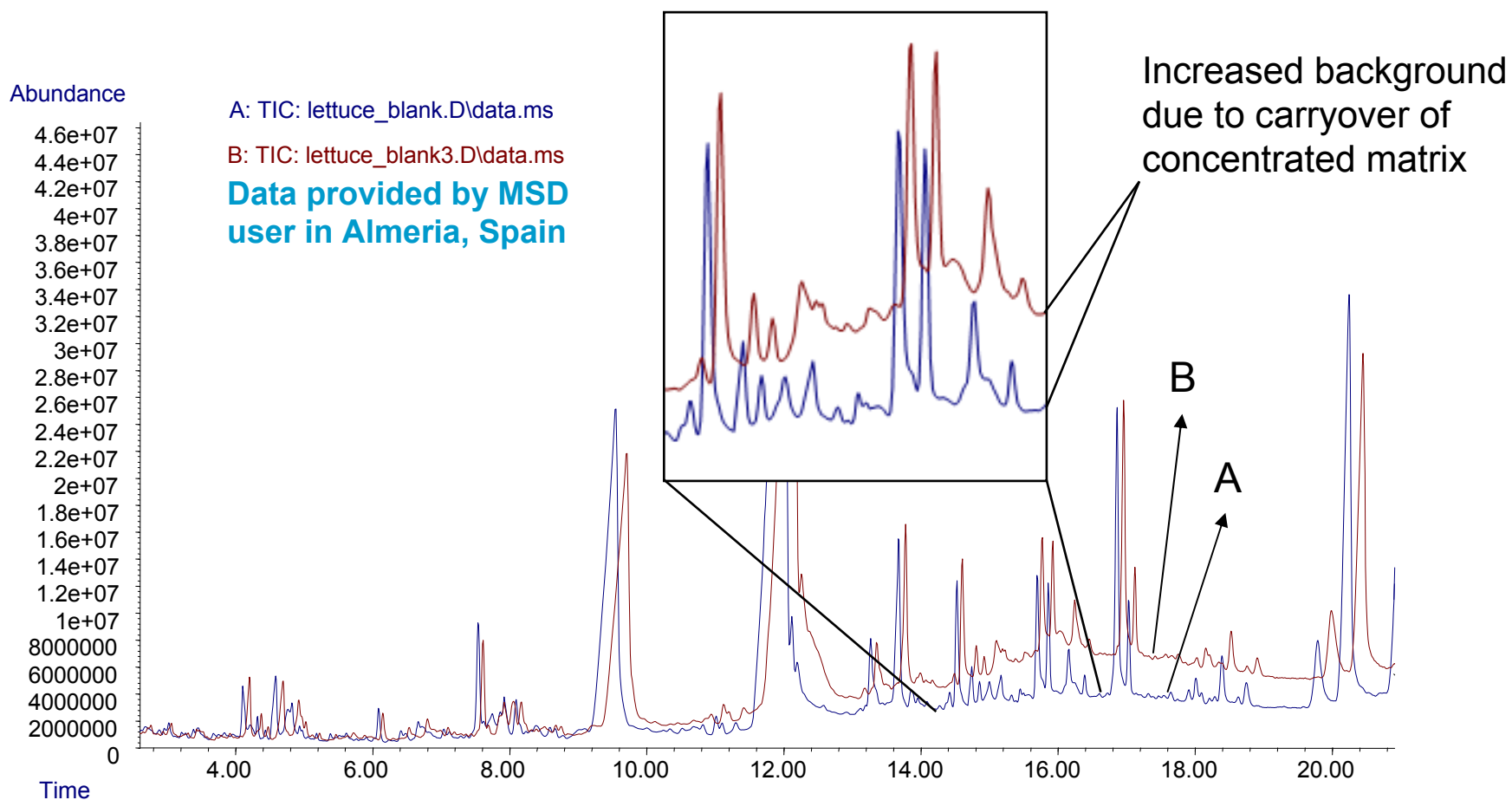
Overlay of two chromatograms of a blank extract injected BEFORE (A) and AFTER (B) three injections without backflush

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Backflush

During GC Run

After GC Run

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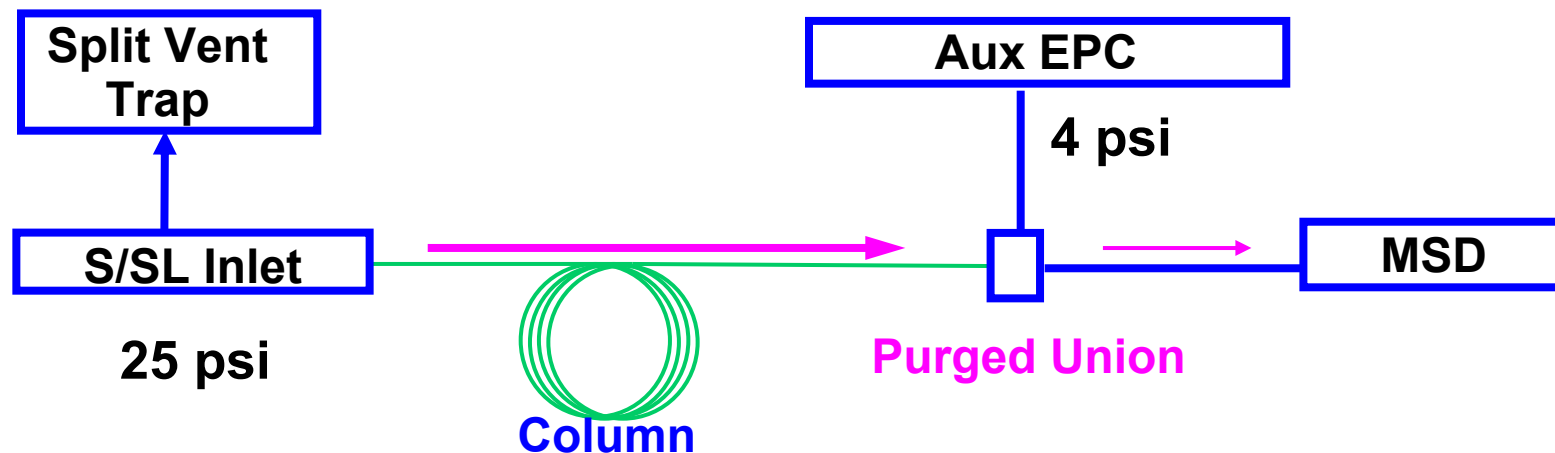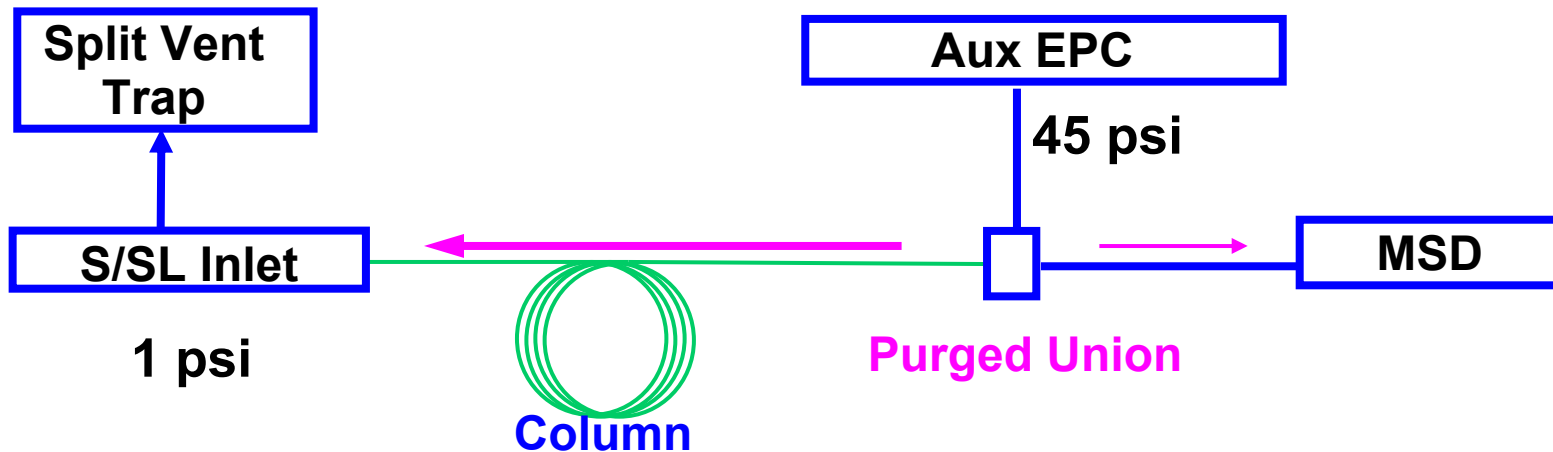
With Backflush: No Increased Background (Less Spectral Noise) and Consistent Retention Times
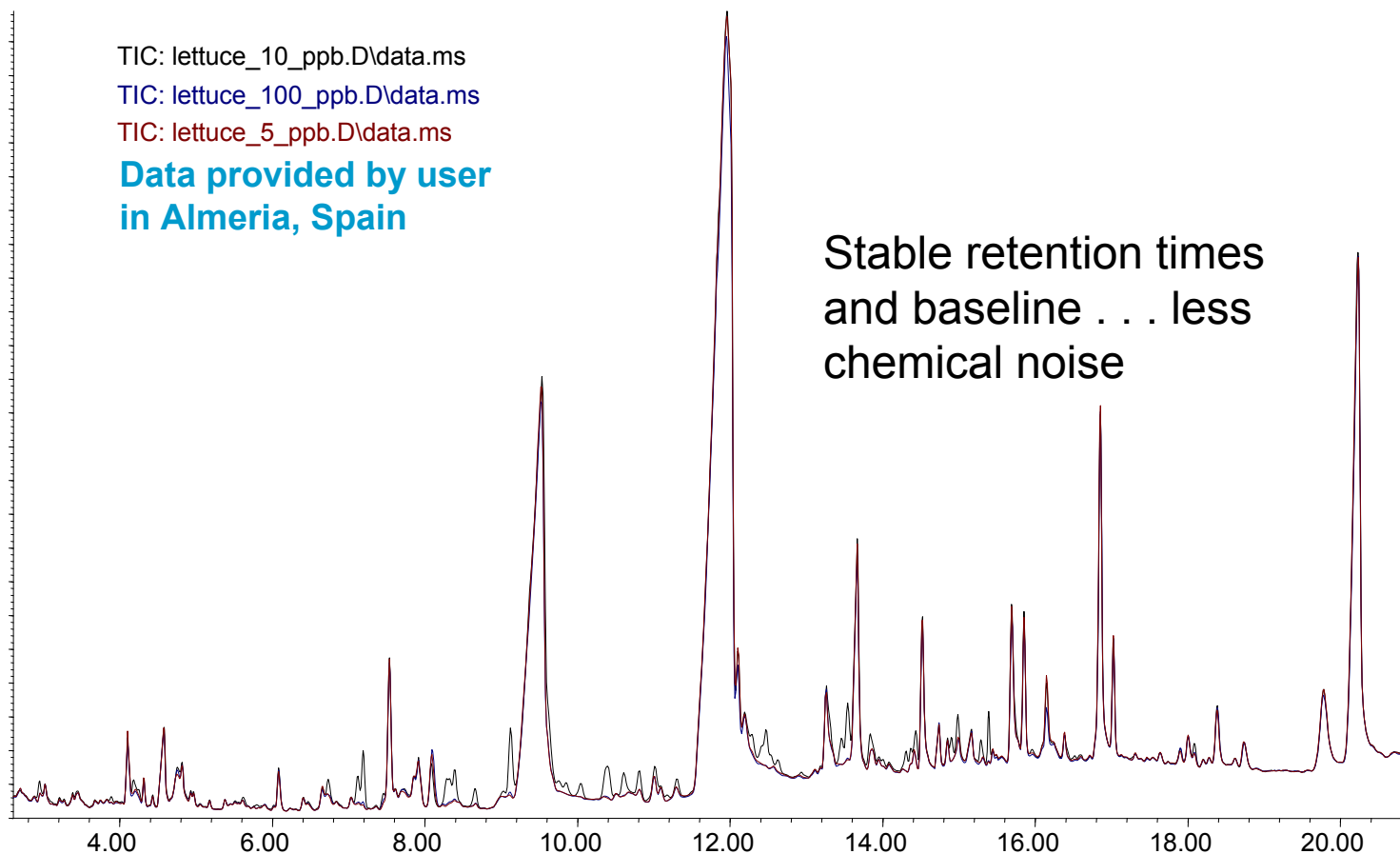
Overlay of three chromatograms of lettuce extract run with 2 min of back flush

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Purged Ultimate Union for GC/MS
New, simple CFT technology for backflush

Vent-less injector and column maintenance (first column)

Improved backflush

- 1/4 the time and/or lower pressure
- Compatible with diffusion pump MSD

Less loss of sensitivity (less flow added = less dilution)

Option of different phase/dimension for each column

Less complex

- Simple GC configuration (existing supplies)
- Setpoints calculated by GC
- Pressure pulsed injections OK
- Constant flow mode easy!!

Purged Ultimate Union

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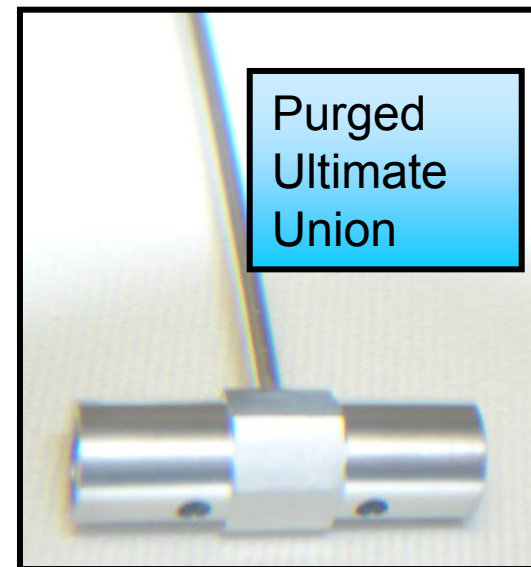
Analytical Reality of GC/MS/MS Methods

GC/MS/MS needs backflush as much or more than GC/MS to avoid "invisible" problems:

source contamination

loss of sensitivity

And to avoid the visible problems:

changing retention times

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Method Building and Optimization Tools for the 7000 Series Triple Quad GC/MS/MS

1. **Dynamic MRM for GC/MS – optimization of MRM method for best analytical performance**
2. **Design Experiment Assistant – Create MRM parameter optimization experiments**
3. **Analyze Experiments Assistant – Automatically analyze MRM optimization experiments**

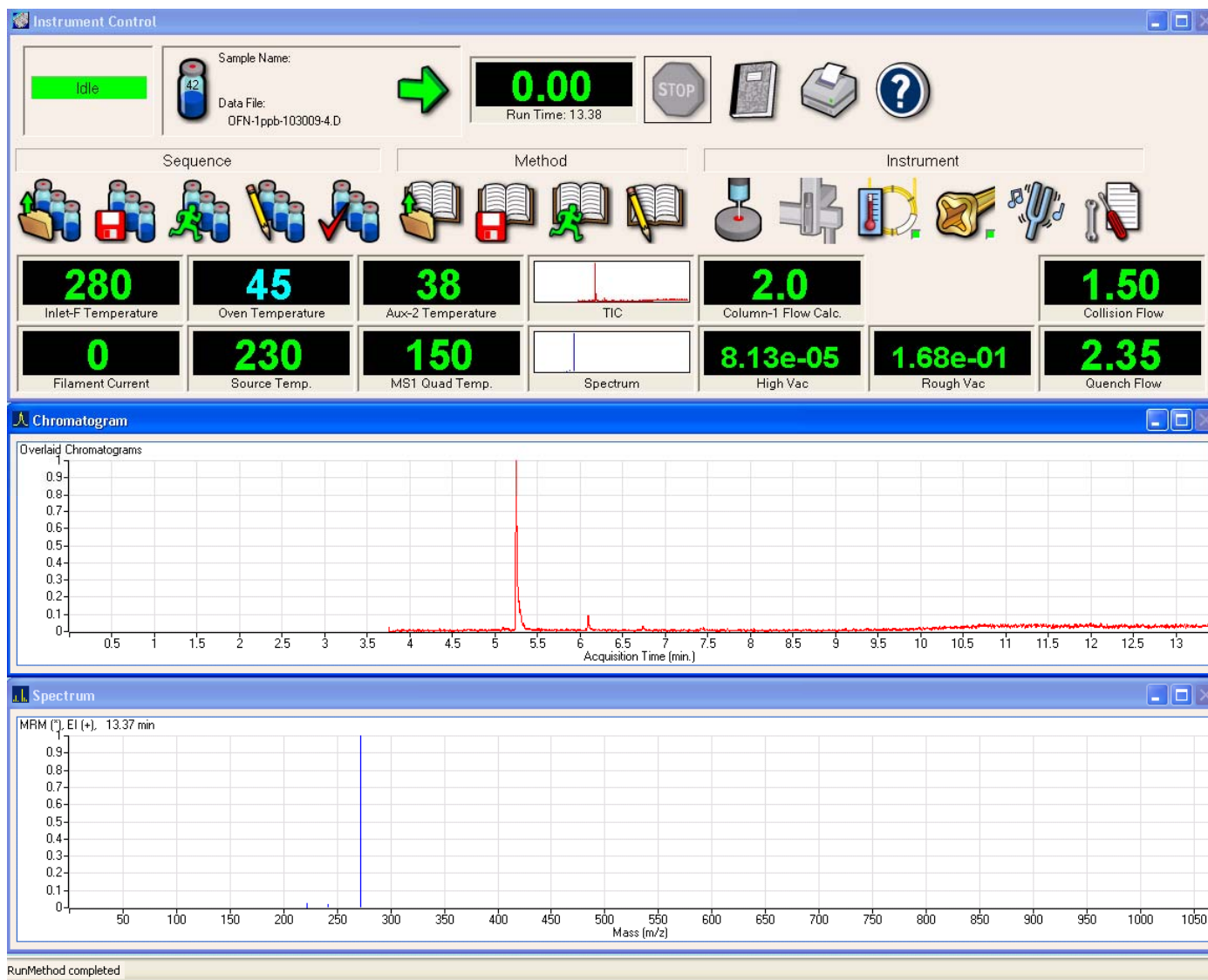Our measure is your success.

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Dynamic MRM Assistant

The Dynamic MRM Assistant optimizes dwell times and time segments for sensitivity.

GC/MS/MS Software Modules

Acquisition

Analysis

Excel Reporting
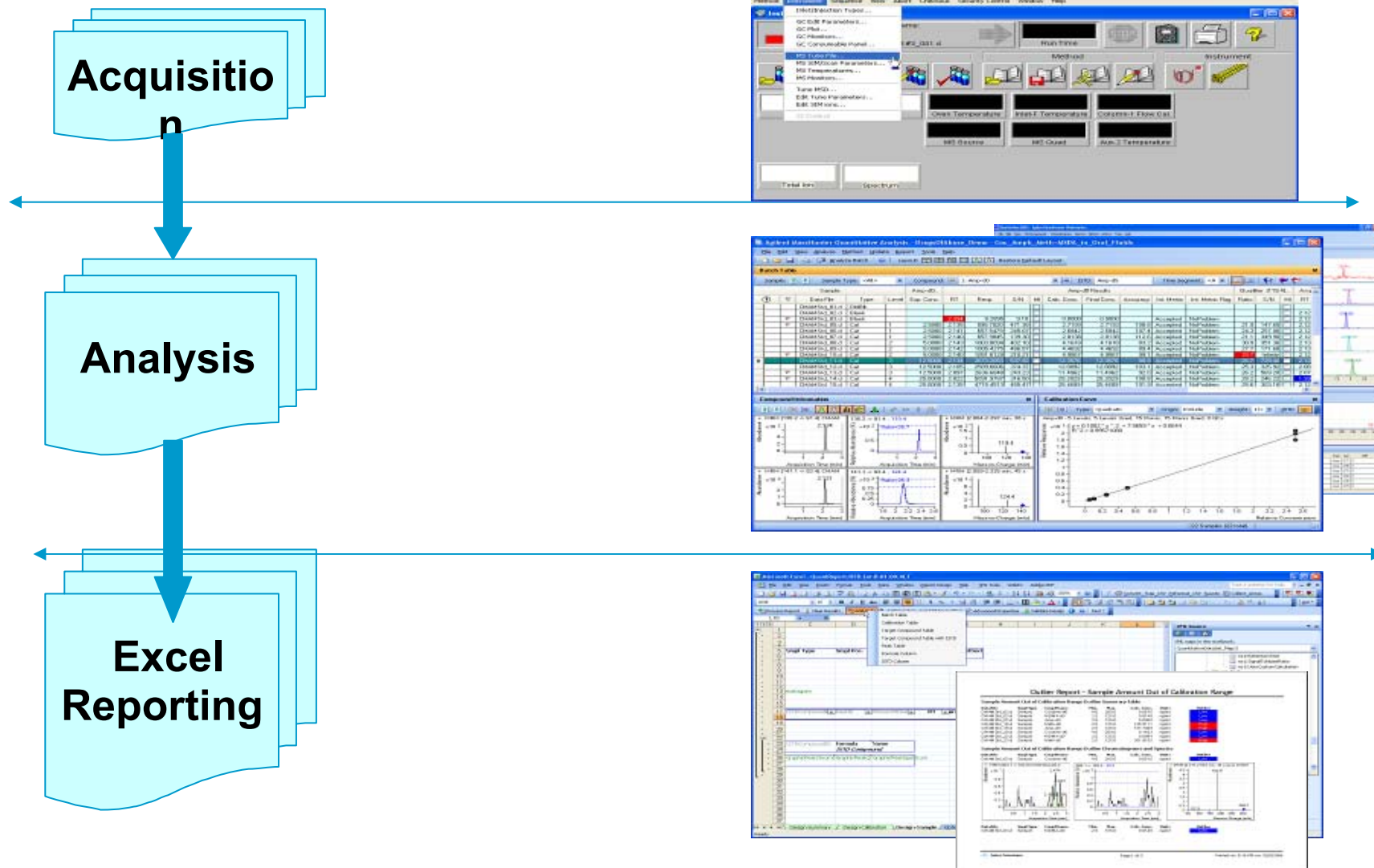
Instrument Control UI/Navigation

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MS/MS Acquisition Method Editor Dialog

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Some GC/MS/MS Applications

- **Pesticides in fruits/veges/marine biota**
- **PCBs**
- **Nitro-PAHs in air particulates**
- **Organo-tins**
- **Melamine in milk and baby formula**
- **Drug Screens**
- **PBDE Flame Retardants**
- **Anabolic Steroids in urine/blood**

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